

## **Revealing Nanoscale Details of Electrochemical Systems Through First-principles Simulations of X-ray Absorption Spectroscopy**

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The inherent complexity of electrochemical systems presents a major bottleneck for advancing current battery technologies towards desirable targets for increased efficiency, reduced cost and improved safety.

Specifically, we often lack quantitative knowledge of the chemical speciation in the electrolyte or at the interface with the electrodes and rely frequently on poorly validated hypotheses to appreciate which of these species are active in electrochemical processes. Using a combination of first-principles molecular dynamics sampling and simulated X-ray absorption spectroscopy, we can provide insight into the atomistic details of various components of an electrochemical system and its interfaces, with validation provided by X-ray absorption spectra measured under the correct working conditions. Examples will be presented with respect to fundamental understanding of electrochemical processes at the nanoscale, and specific applications to beyond Li-ion technologies, such as lithium-sulfur and magnesium-ion batteries.